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NEWS
                Web Page URLs for STN Seminar Schedule - N. America
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                "Ask CAS" for self-help around the clock
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                CASREACT(R) - Over 10 million reactions available
NEWS 4 DEC 14 2006 MeSH terms loaded in MEDLINE/LMEDLINE
NEWS 5
        DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
        DEC 14 CA/CAplus to be enhanced with updated IPC codes
NEWS 6
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                New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
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NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV
NEWS 13 JAN 30 Saved answer limit increased
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency
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NEWS 15 FEB 21
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NEWS 16 FEB 22
                Status of current WO (PCT) information on STN
NEWS 17 FEB 22
                The IPC thesaurus added to additional patent databases on STN
NEWS 18 FEB 22 Updates in EPFULL; IPC 8 enhancements added
NEWS EXPRESS
             FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
             CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
             AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
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http://download.cas.org/express/v8.0-Discover/

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FILE 'HOME' ENTERED AT 09:44:18 ON 28 FEB 2006

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10817532.str

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exact/norm bonds:

2-19 3-14 4-20 5-15 6-22 8-23 10-24 11-16 12-25

exact bonds :

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G1:H,Ak

Match level:

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

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G1 H, Ak

Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED 4 ITERATIONS 1 ANSWERS

1 TO

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

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PROJECTED ANSWERS:

L2 1 SEA SSS SAM L1

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167.15

FILE 'CAPLUS' ENTERED AT 09:45:02 ON 28 FEB 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2002:575783 CAPLUS

DOCUMENT NUMBER:

137:125048

TITLE:

Preparation of compounds which mimic the chemical and

biological properties of discodermolide

INVENTOR(S):

Smith, Amos B.; Beauchamp, Thomas J.; Lamarche,

Matthew J.

PATENT ASSIGNEE(S):

The Trustees of The University of Pennsylvania, USA U.S. Pat. Appl. Publ., 127 pp., Cont.-in-part of U.S.

SOURCE: U.S. Pat. Appl. P Ser. No. 455,649.

CODEN: USXXCO

DOCUMENT TYPE:

 ${\tt Patent}$ 

LANGUAGE:

English

6

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OTHER SOURCE(S):
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GΙ

MARPAT 137:125048

AΒ Discodermolide analogs, such as I [R = H, OR33; X = H2, O; R4, R9, R33 = H, acid labile protecting group; R25 = H, oxidatively labile protecting group; R16, R32 = H, alkyl], were prepared Synthetic routes to both (-)and (+)-discodermolide were presented.

Ι

IT 252342-54-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of compds. which mimic the chemical and biol. properties of discodermolide)

RN 252342-54-4 CAPLUS CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

• I-

REFERENCE COUNT:

THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2002:449643 CAPLUS

DOCUMENT NUMBER:

137:33164

TITLE:

Preparation of compounds which mimic the chemical and

biological properties of discodermolide

INVENTOR(S):

Smith, Amos B., III; Beauchamp, Thomas J.; Lamarche,

Matthew J.

PATENT ASSIGNEE(S):

The Trustees of the University of Pennsylvania Center

for Technology Transfer, USA

SOURCE:

PCT Int. Appl., 267 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

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OTHER SOURCE(S):
                         MARPAT 137:33164
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AB Discodermolide analogs, such as I [R = H, OR33; X = H2, O; R4, R9, R33 = H, acid labile protecting group; R25 = H, oxidatively labile protecting group; R16, R32 = H, alkyl], were prepared Synthetic routes to both (-)-and (+)-discodermolide were presented.

I.

IT 252342-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of compds. which mimic the chemical and biol. properties of discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

D<sub>I</sub>-

ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2002:123244 CAPLUS

DOCUMENT NUMBER: TITLE:

136:183657 Process for the biomediated preparation of

intermediates for use in the synthesis of polyketides,

such as epothilone D and discodermolide

INVENTOR(S):

Santi, Daniel V.; Ashley, Gary; Myles, David C.

PATENT ASSIGNEE(S):

Kosan Biosciences, Inc., USA PCT Int. Appl., 129 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

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OTHER SOURCE(S):
                         CASREACT 136:183657; MARPAT 136:183657
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GI

Ι

AB The present invention relates to compds., such as I, made by a subset of modules from one or more polyketide synthase ("PKS") genes that are used as starting material in the chemical synthesis of novel mols., particularly naturally occurring polyketides or derivs. thereof. The biol. derived intermediates ("bio-intermediates") generally represent particularly difficult compds. to synthesize using traditional chemical approaches due to one or more stereocenters. In one aspect of the invention, an intermediate in the synthesis of epothilone is provided that feeds into the synthetic protocol of Danishefsky and co-workers. In another aspect of the invention, intermediates in the synthesis of discodermolide are provided that feed into the synthetic protocol of Smith and co-workers. By taking advantage of the inherent stereochem. specificity of biol. processes, the syntheses of key intermediates and thus the overall syntheses of compds. like epothilone and discodermolide are greatly simplified.

## IT 252342-54-4P

RN

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (process for the biomediated preparation of intermediates for use in the synthesis of polyketides, such as epothilone D and discodermolide) 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

• I-

L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2001:412212 CAPLUS

DOCUMENT NUMBER: TITLE:

135:19496

Preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone

derivatives for pharmaceutical use

INVENTOR(S):

Smith, Iii Amos B.; Beauchamp, Thomas J.; Lamarche,

Matthew J.; Arimoto, Hirokazu

PATENT ASSIGNEE(S):

The Trustees of the University of Pennsylvania, USA

U.S., 126 pp., 6096904 Cont.-in-part of U.S.

6,096,904. CODEN: USXXAM

DOCUMENT TYPE:

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LANGUAGE:

SOURCE:

English

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CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
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PRIORITY APPLN. INFO.:
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                                            US 1998-21878
                                                                 A1 19980211
                                            US 1998-121551
                                                                A2 19980723
                                            US 1999-455649
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                                            US 2004-779049
                                                                   20040213
                                                                Α
OTHER SOURCE(S):
                         CASREACT 135:19496; MARPAT 135:19496
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GΙ

R140 COR16 R150 Me R150 CHO

R12 O I SEt III

$$H_2C$$
  $R^1$   $R^2$   $R^3$   $R^6$   $R^6$   $R^8$   $R^8$ 

Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid AB labile protecting groups; R16 = H, alkyl] and II [R1, R2, R7, R8 = alkyl; R3, R6, R16 = H, alkyl; R4, R9 = acid labile hydroxyl protecting group; R25 = oxidatively labile hydroxyl protecting group; X = :C(J)R16, a Wittigolefination formed from a pyranylalkyl ketone, such as I and II (X = P+Ph3I-)], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon III (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2-methylpropanoic acid Me ester. The synthetic utility of II was subsequently demonstrated by its use in the preparation of (-)-discodermolide.

## IT 252342-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN252342-54-4 CAPLUS

Phosphonium, [(2R, 3R, 4S, 5Z, 8S, 9R, 10R, 11S, 12S, 13Z)-3, 9-bis[[(1,1-CN dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

I-

REFERENCE COUNT:

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

30

ACCESSION NUMBER:

2000:597937 CAPLUS

DOCUMENT NUMBER:

133:335118

TITLE:

Evolution of a Gram-Scale Synthesis of (+)-Discodermolide

Smith, Amos B., III; Beauchamp, Thomas J.; LaMarche,

AUTHOR(S):

Matthew J.; Kaufman, Michael D.; Qiu, Yuping; Arimoto,

Hirokazu; Jones, David R.; Kobayashi, Kaoru

CORPORATE SOURCE:

Department of Chemistry Monell Chemical Senses Center

and Laboratory for Research on the Structure of

Matter, University of Pennsylvania, Philadelphia, PA,

19104, USA

SOURCE:

Journal of the American Chemical Society (2000

), 122(36), 8654-8664

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 133:335118

GI

AB An efficient, highly convergent, stereocontrolled total synthesis of the potent antimitotic agent (+)-discodermolide (I) has been achieved on gram scale. Key elements of the successful strategy include (1) elaboration of three advanced fragments from a common precursor (CP) which embodies the repeating stereochem. triad of the discodermolide backbone, (2) \u03c4-bond installation of the Z trisubstituted olefin, exploiting a modified Negishi cross-coupling reaction, (3) synthesis of a late-stage phosphonium salt utilizing high pressure, and (4) Wittig installation of the Z disubstituted olefin and the terminal (Z)-diene.

IT 252342-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(evolution of a gram-scale synthesis of (+)-discodermolide)

RN 252342-54-4 CAPLUS

CN Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

## THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:531688 CAPLUS

133:135166

DOCUMENT NUMBER: TITLE:

Preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone

derivatives for pharmaceutical use

INVENTOR(S):

Smith, Amos B., III; Qiu, Yuping; Kaufman, Michael; Arimoto, Hirokazu; Jones, David R.; Kobayashi, Kaoru;

Beauchamp, Thomas J.

PATENT ASSIGNEE(S):

The Trustees of the University of Pennsylvania, USA

SOURCE:

U.S., 83 pp., Cont.-in-part of U.S. 5,789,605.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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EP	1105						2001											
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OMILED C							122			US 2	004-	7790	49		A 2	0040	213	

OTHER SOURCE(S): MARPAT 133:135166

GI

$$R^{140}$$
  $COR^{16}$   $R^{150}$   $R^{$ 

AB Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid labile protecting groups; R16 = H, alkyl], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon II (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2methylpropanoic acid Me ester. The synthetic utility of II was subsequently demonstrated by its use in the preparation of (-)-discodermolide.

IT 252342-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN

252342-54-4 CAPLUS Phosphonium, [(2R, 3R, 4S, 5Z, 8S, 9R, 10R, 11S, 12S, 13Z)-3, 9-bis[[(1,1-CN dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

) I-

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:84572 CAPLUS

DOCUMENT NUMBER: 132:137207

TITLE: Preparation of intermediates for the synthesis of

discodermolides and their polyhydroxy dienyl lactone

derivatives for pharmaceutical use

INVENTOR(S): Smith, Amos B. Iii; Qiu, Yuping; Kaufman, Michael;

Arimoto, Hirokazu; Jones, David R.; Kobayashi, Kaoru;

Beauchamp, Thomas J.

PATENT ASSIGNEE(S):

The Trustees of the University of Pennsylvania, USA

PCT Int. Appl., 201 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

SOURCE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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	2000	0048	65		A2 20000203 A3 20000921				WO 1999-US16369						19990720 <			
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AU	9952	190			<b>A</b> 1		2000	0214		AU 1	999-	5219	0		1	9990	720 <	<
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									US 1996-759817 WO 1999-US16369									
										US 2	004-	1190	49	A 20040213				

OTHER SOURCE(S):

MARPAT 132:137207

GΙ

$$R^{140}$$
  $COR^{16}$   $R^{140}$   $CHO$   $R^{150}$   $R^{150}$ 

AB Preparation of intermediates, such as I [R11, R12 = alkyl; R14, R15 = acid labile protecting groups; R16 = H, alkyl], for the synthesis of discodermolides and their analogs, which are useful as pharmaceuticals, was presented. Thus, synthon II (R14 = R15 = SiMe2CMe3) was prepared via a multistep synthetic sequence starting from (2R)-3-hydroxy-2-methylpropanoic acid Me ester. The synthetic utility of II was

subsequently demonstrated by its use in the preparation of (-)-discodermolide.

IT 252342-54-4P

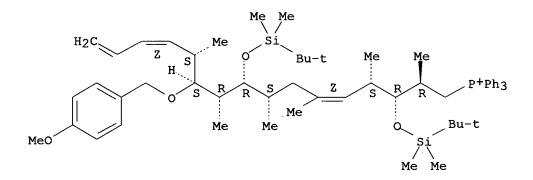
> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of intermediates for the synthesis of discodermolides and their polyhydroxy dienyl lactone derivs. for pharmaceutical use)

RN252342-54-4 CAPLUS

Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-CN dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.



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ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN L5

1999:694867 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:35548

TITLE: Gram-Scale Synthesis of (+)-Discodermolide

AUTHOR(S): Smith, Amos B., III; Kaufman, Michael D.; Beauchamp,

Thomas J.; LaMarche, Matthew J.; Arimoto, Hirokazu

CORPORATE SOURCE: Department of Chemistry Monell Chemical Senses Center

and Laboratory for Research on the Structure of

Matter, University of Pennsylvania, PA, 19104, USA

SOURCE: Organic Letters (1999), 1(11), 1823-1826

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

A triply convergent, highly efficient second-generation synthesis of the potent antimitotic agent (+)-discodermolide has been achieved on a 1-q scale.

ΙT 252342-54-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(gram-scale synthesis of (+)-discodermolide)

RN 252342-54-4 CAPLUS

Phosphonium, [(2R,3R,4S,5Z,8S,9R,10R,11S,12S,13Z)-3,9-bis[[(1,1-CN dimethylethyl)dimethylsilyl]oxy]-11-[(4-methoxyphenyl)methoxy]-2,4,6,8,10,12-hexamethyl-5,13,15-hexadecatrienyl]triphenyl-, iodide (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

• I-

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 09:44:18 ON 28 FEB 2006)

FILE 'REGISTRY' ENTERED AT 09:44:27 ON 28 FEB 2006

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 14 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:45:02 ON 28 FEB 2006

L4 18 S L3 FULL

L5 8 S L4 AND PY<2003

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	ENTRY	SESSION
FULL ESTIMATED COST	43.29	210.44
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-6.00	-6.00

STN INTERNATIONAL LOGOFF AT 09:45:48 ON 28 FEB 2006